General Recommendations of Particle Speciation for Class I Visibility Analyses

Introduction & Overview

This report is intended to provide general guidance to CALPUFF model users and reviewers regarding methods to estimate the particle species profile for use in Class I modeling analyses for possible visibility impairment.

The particle speciation profile is intended to represent the source particulate matter (PM) emissions in terms of those species that contribute to visibility impairment. PM emissions can contribute to visibility impairment as follows:

Emitted PM Species	Light Extinction Coefficient
Coarse PM (CPM)	0.6
Fine PM (FPM)	1.0
Sulfate (SO_4)	3.0 * f(RH)
Secondary Organic Aerosol (SOA)	4.0
Elemental Carbon (EC)	10.0

Because different PM material exhibits varying characteristics when it comes to visibility impairment, the PM emissions must reflect the different species in the modeled emissions. The recommendations below are an attempt to provide this information for the CALPUFF model emission inputs.

General Recommendations and Rationale

In general, the sum of all PM species (CPM + FPM + SO4 + SOA + EC) should equal the allowable PM-10 emission rate requested by the applicant in the permit application. A discussion on development of the emissions for each species is provided below. The PM speciation profile relies principally on knowledge of the “filterable” (front-half) and “condensable” (back-half) emissions information available in EPA documents such as AP-42. Also, the PM speciation profile is normally applied only to larger combustion sources in the CALPUFF modeling. Minor PM sources usually do not contribute significantly to visibility impairment and any errors caused by not including a PM speciation profile would be small. Also, non-combustion PM emissions would not be expected to have a significant carbonaceous component.

Sulfate (SO_4)

SO_4 emissions represent the "primary" sulfate that is released to the atmosphere. In particular, where ammonia injection systems such as selective catalytic reduction (SCR) are being employed on combustion sources for nitrogen oxide (NOx) emissions control, it is believed that some of the ammonia may combine with the sulfur emissions to form ammonium sulfate at the stack. Since SO_4 is a potentially significant contributor to visibility, these emissions should be modeled in CALPUFF for sources where they are believed to be significant.

In cases where the applicant has estimated the H_2SO_4 (sulfuric acid mist) emissions, or if similar data are listed in AP-42, these data can be used as an estimate of the primary SO_4 emissions.

Otherwise, it is usually assumed that a fraction of the fuel sulfur may be converted to SO_4, rather than assuming 100% conversion to SO_2.

Since the applicant has included some of the fuel sulfur as SO_4 emissions when following this approach, it is acceptable for the CALPUFF visibility modeling that the sulfur included as primary SO_4 emissions be deducted from the facility SO_2 emissions in CALPUFF. However, for PSD increment modeling, it is generally preferred to retain all of the fuel sulfur as SO_2 in the CALPUFF emissions.

Elemental Carbon (EC)

EC represents the unburned carbon that passes through a fuel combustion unit. For gaseous-fuel sources such as natural gas boilers, combustion turbines, etc.), it is reasonable to assume that 100% of the "filterable" PM emissions are unburned fuel, and as such would be characterized as EC.

The EC component of the "filterable" PM emissions for liquid-fuel or solid fuel combustion sources would be much smaller because of the contribution of inorganic ash to the total PM load at such sources. Very few sources have data on the percentage of carbon in the filterable PM mass exiting the stack. In the absence of such data, it is normally assumed that only a small fraction of the filterable PM mass (5% or less) would be EC, with the remainder being inorganic ash. Additional data on the carbon content of collected PM mass of liquid and solid-fuel boilers can be used to help refine this initial estimated for EC.

Secondary Organic Aerosol (SOA)

SOA is assumed to be represented by the "organic" fraction of any condensable PM emissions.

For many combustion source types, AP-42 lists the condensable PM emissions (CPM) by the “organic” and “inorganic” fractions of the back-half PM catch. The fraction of PM mass in the “organic” fraction of the CPM are assumed to be SOA. For example, AP-42 Table 1.1-5 lists 20% of the CPM from coal combustion is “organic”. So, the SOA at a pulverized coal combustion unit is estimated as 20% of the CPM emissions.

In the case of gaseous fuel combustion sources, it is assumed that all of the condensable PM mass is either SOA or sulfate (SO_4). So, the SOA is determined for a gaseous fuel source by subtracting the SO_4 emissions from the CPM emissions.

Fine and Coarse Particulate Matter (PMF and PMC)

The PM emissions not otherwise assigned to SO_4, EC, or SOA are assumed to be inorganic and are therefore PMF or PMC. Where PMF and PMC are separated by particle size, the breakpoint used should be 2.5 microns.

All CPM emissions not otherwise assigned to SO_4 or SOA should be listed as PMF as it is reasonable to assume that all condensable PM emissions are less than 2.5 microns in size. In the absence of any evidence to the contrary, it is also reasonable to assume that all PM-10 emissions are PMF for gaseous fuel combustion sources.

Where particle size data exist for a particular fuel combustion source, it may be possible to split the PM-10 emissions into the PMF and PMC fractions. However, the size data (i.e. AP-42) generally can be applied only to the filterable PM mass. For example, particle size data for different types of pulverized coal combustion are listed in Table 1.1-6 through 1.1-11 of AP-42.

Also, where particle size data are available for non-combustion sources, these can also be used to separate PMF and PMC at the discretion of the user.

In many cases, all of the inorganic PM-10 emissions are all assigned as PMF, which would be the worst-case from a visibility impact perspective.

Sample PM Speciation Profiles

The attached table summarizes some of the Pm speciation profiles developed for common source categories. These should be considered recommendations only. Where the user has site-specific information on emissions that would generate a different result, these data should be used in lieu of the generalized recommendations.

Generalized CALPUFF PM Speciation Profiles
for Selected Emission Source Categories

Source Category	Filterable vs. Condensable		Recommended PM Profile				
	Filterable	Condensable (CPM)	SO_4 (See Notes 1 & 2)	EC	SOA	PMF	PMC
Natural-Gas Fired Combustion Turbine	0.25	0.75	Site-specific data, or 0.33*SO_2	0.25	CPM-SO_4	0.0	0.0
Oil-Fired Combustion Turbine	0.37	0.63	Site-specific data, or 0.4*SO_2	0.185	CPM-SO_4	0.185	0.0
Circulating Fluidized Bed Boiler (coal-fired)	0.2	0.8	Site-specific data, or 0.64	0.01	0.16	0.08+CPM-SOA-SO_4	0.11
Lime Kilns	0.28	0.72	Site-specific data, or 0.63	0.01	0.09	0.07+ CPM-SOA-SO_4	0.20
Cement Kilns (dry kiln with fabric filter)	0.14	0.86	Site-specific data, or 0.76	0.01	0.10	0.13 +CPM-SOA-SO_4	0.0
Pulverized Coal (dry bottom with fabric filter)	0.5	0.5	Site specific data, or 0.4	0.01	0.10	0.245 +CPM-SOA-SO_4	0.245

Note 1: SO_4 should be adjusted to account for the molecular weight difference between SO_2 and SO_4 (96/64).

Note 2: SO_4 assumed to be 100% of inorganic CPM unless site-specific data indicates otherwise.